Measurable Consequences of the Local Breakdown of the Concept of Temperature

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Abstract. – Local temperature defined by a local canonical state of the respective subsystem, does not always exist in quantum many body systems. Here, we give some examples of how this breakdown of the temperature concept on small length scales might be observed in experiments: Measurements of magnetic properties of an anti-ferromagnetic spin-1 chain. We show that those magnetic properties are in fact strictly local. As a consequence their measurement reveals whether the local (reduced) state can be thermal. If it is, a temperature may be associated to the measurement results, while this would lead to inconsistencies otherwise.

With the advent of nanotechnology, the applicability of thermodynamics on small length scales has become an important subject of current research. There has been substantial progress in the fabrication and processing of nanostructures, e.g. carbon nanotubes [1], and measurements of thermal properties on the corresponding scales are becoming possible [2]. However, despite this amazing experimental advances, the theoretical foundation of thermodynamics on small scales remains unclear [3,4]. First attempts to generalize thermodynamics such that it would apply to small systems date back to the sixties and are receiving increasing attention today [5,6].

Recently [7–9], Hartmann, Mahler and Hess gave a first quantitative estimate of the length scales, below which the standard concept of temperature ceases to exist. They considered a large chain of particles with nearest neighbor interactions, which was assumed to be in a thermal, i.e. canonical, state. In this scenario, subgroups of N adjacent particles are in a canonical state if N is larger than a threshold value $N_{\min}$ which depends on the global temperature, $N_{\min} = N_{\min}(T)$. The reduced density matrix of a subgroup deviates from the canonical form if $N < N_{\min}$. The temperature dependence of $N_{\min}$ is as follows: The lower the temperature, the larger $N_{\min}$, i.e. the larger the groups need to be. In other words, for each group size N, there is a threshold temperature above which the groups are in a canonical state and below they are not. The predicted length scales depend on the definition of temperature

used. In [8] and [9], local temperature has been defined to exist if the respective part of the system is in a canonical state.

Why should we care about the non-existence of local temperature? There are at least three situations for which this possibility needs special attention: One obvious scenario refers to the limit of spatial resolution on which a temperature profile could be defined. However a spatially varying temperature calls for non-equilibrium - a complication which we will exclude here. A second application deals with partitions on the nanoscale: If a modular system in thermal equilibrium is partitioned into two pieces, say, the two pieces need no longer be in a canonical state, let alone have the same local temperature.

Temperature is always measured indirectly via observables, which, in quantum mechanics, are represented by hermitian operators. Usually, one is interested in measuring the temperature of a system in a stationary state. The chosen observable should therefore be a conserved quantity, i.e. its operator should commute with the Hamiltonian of the system.

A conventional technique, e.g., is to bring the piece of matter, the temperature T of which is to be measured, in thermal contact with a box (volume V) of an ideal gas (number of particles n) and to measure the pressure p of the gas, which is related to its temperature by $n\,k_B\,T = p\,V$ (k_B is Boltzmann's constant). Since the gas is in thermal equilibrium with the considered piece of matter, both substances have the same temperature. A measurement of p for constant V allows to infer the global temperature T of the piece of matter.

Such a thermometer functions as long as it does not significantly perturb the measured object (weak coupling), irrespective of whether its coupling to the object is local or not. One might thus doubt whether a local temperature can be measured at all. System bath models show that the system always relaxes to a canonical state with the global temperature of the bath, no matter how localized the system bath interaction might be [10]. However, there are examples, where a local application of Boltzmann-Gibbs thermostatistics is known to fail due to strong correlations [11, 12].

Here, we consider observables of the object itself, which can be used to measure local temperatures T_{loc}, i.e. temperatures of subsystems, provided the subsystems are in a canonical state. In turn, if the respective subsystems are not in a canonical state, this fact should modify the measurement results for those observables. For systems composed of weakly interacting subsystems, which are in a thermal state, the total state factors with respect to the subsystems and the subsystems themselves are also in thermal states, i.e. local temperature exists. For strongly interacting subsystems, however, local temperatures cease to exist due to correlations between subsystems. Note that, if the system reached its thermal state via interaction with a bath, the coupling to the latter must be weak, otherwise the state of the entire system can, in general, not be thermal [4, 10].

Pertinent systems, for which such effects can easily by studied, are magnetic materials. As we will demonstrate below, properties of single spins can be infered from measurements of even macroscopic magnetic observables. These materials thus allow to study the existence of temperature, as defined by the existence of a canonical state, on the most local scale possible, i.e. for single spins.

As our model, we consider a homogeneous chain of spin-1 particles interacting with their nearest neighbors. For the interactions, we assume a Heisenberg model. The Hamiltonian of this system reads [13]:

$$H = B \sum_{j=1}^{n} \sigma_j^z + J \sum_{j=1}^{n} \vec{\sigma}_j \cdot \vec{\sigma}_{j+1}, \tag{1}$$

where $\vec{\sigma}_j = (\sigma_j^x, \sigma_j^y, \sigma_j^z)$ and $\vec{\sigma}_j \cdot \vec{\sigma}_k = \sigma_j^x \sigma_k^x + \sigma_j^y \sigma_k^y + \sigma_j^z \sigma_k^z$. σ_j^x, σ_j^y and σ_j^z are the spin-1 matrices. B is an applied magnetic field, J the coupling and n the number of spins. The

coupling J is taken to be positive, $J > 0$. The spins thus tend to align anti-parallel and the material is anti-ferromagnetic. The local Hamiltonian of subsystem j is $H_j = B\,\sigma_j^z$. The system has periodic boundary conditions and is thus translation invariant.

We assume that the system (1) is in a thermal state,

$$\rho = \frac{1}{Z}\,\exp\left(-\frac{H}{k_B\,T}\right), \tag{2}$$

where T is the temperature and Z the partition sum. The interaction of this system to a possible heat bath acting as a thermostat must be weak [4,10]. Note that the temperature T is a global property of the system since it is defined in the eigenbasis. The eigenstates do not factorize with respect to single spins and therefore have non-local properties.

The reduced density operator of subsystem j may be represented in the eigenbasis of the respective subsystem Hamiltonian, H_j; let its diagonal matrix elements be p_α. It is convenient to introduce a spectral temperature T_{spec}, which would coincide with T_{loc} if the local state was canonical but which formally exists for any state:

$$\frac{1}{T_{\text{spec}}} \equiv -k_B \sum_{\alpha > 0} \frac{p_\alpha}{1 - p_0}\,\frac{\ln(p_\alpha) - \ln(p_0)}{E_\alpha - E_0}. \tag{3}$$

Here the E_α are the spectrum of the isolated subsystem; E_0 denotes the ground state. The factor $(1 - p_0)^{-1}$ is the normalization. The local state may be characterized by T_{spec} and a parameter Δ describing mean relative square deviations of the occupation probabilities p_α from those of a canonical state, p_α^c, with $T_{\text{loc}} = T_{\text{spec}}$,

$$\Delta^2 \equiv \sum_\alpha p_\alpha \left(\frac{p_\alpha - p_\alpha^c}{p_\alpha}\right)^2, \tag{4}$$

where $p_\alpha^c = \exp\left(-E_\alpha/k_B\,T_{\text{spec}}\right)/\sum_\alpha \exp\left(-E_\alpha/k_B\,T_{\text{spec}}\right)$. Note that T_{spec} and Δ depend on the global temperature T **and** the type and strength of subsystem interactions. T_{spec} and Δ do, of course, not fully characterize the local state (this would require 8 real numbers), they merely classify it in a pertinent way.

Figure 1 shows the spectral temperature T_{spec}, the global temperature T and the deviations Δ of the local state from a canonical state with T_{spec} as a function of T for a spin-1 chain of 4 particles with the Hamiltonian (1). While the deviations Δ are small at high T, they become larger for low T, where the spectral temperature T_{spec} starts to rise again as T is lowered further. For $T = 0$, Δ vanishes, since a completely mixed state corresponds to a canonical one with $T_{\text{spec}} \to \infty$. A signature of these local deviations from a canonical state ($\Delta \neq 0$) can be measured.

As an example of such an experiment, we will now consider two different magnetic observables of a spin-1 system with the Hamiltonian (1). The first observable is the magnetization in the direction of the applied field, m_z, which we define to be the total magnetic moment per particle:

$$m_z \equiv \frac{1}{n}\left\langle \sum_{j=1}^{n} \sigma_j^z \right\rangle, \tag{5}$$

where $\langle \mathcal{O} \rangle$ is the expectation value of the operator $\mathcal{O}$, i.e. $\langle \mathcal{O} \rangle = \text{Tr}(\rho\,\mathcal{O})$. In the translation invariant state ρ, the reduced density matrices of all individual spins are equal, and the magnetization (5) can be written as
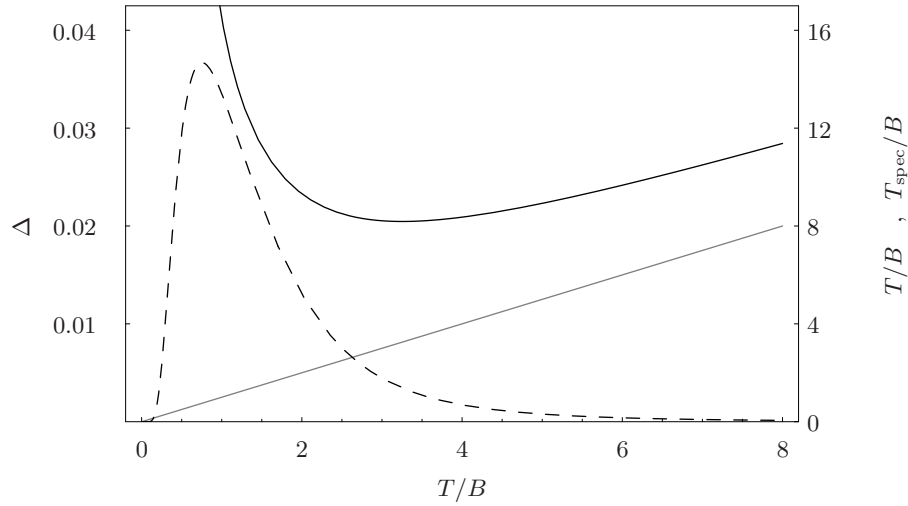
$$m_z = \langle \sigma_k^z \rangle, \tag{6}$$

Fig. 1 – T_{spec} (solid line), T (gray line) and Δ (dashed line) as a function of temperature T for spin-1 chain of 4 particles. T_{spec} and T are given in units of B and $J = 2 \times B$.

for any $k = 1, 2, \ldots, n$. The magnetization, although defined macroscopically, is thus actually a property of a single spin, i.e. a strictly local property.

As our second observable we choose the occupation probability, p, of the $s_z = 0$ level (averaged over all spins),

$$p \equiv \frac{1}{n} \left\langle \sum_{j=1}^{n} |0_j\rangle \langle 0_j| \right\rangle = \langle |0_k\rangle \langle 0_k| \rangle , \tag{7}$$

where the second equality holds for the same reasons as for m_z for any $k = 1, 2, \ldots, n$. p is thus strictly local, too.

Now, if each single spin was in a canonical state with $\Delta = 0$ and a temperature $T_{\text{loc}} = T_{\text{spec}}$, m_z and p would both have to be monotonic functions of T_{loc}. Consequently, T_{loc} could, after calibration, be infered from measurements of m_z or p. Note, that m_z is proportional to the local energy, the average energy of one subsystem.

Figure 2, shows m_z and p as a function of the global temperature T for a spin-1 chain of 4 particles with the Hamiltonian (1) for weak interactions, $J = 0.1 \times B$. Both quantities are monotonic functions of each other. The situation changes drastically when the spins are strongly coupled. In this case the concept of temperature breaks down locally due to correlations of each single spin with its environment. Figure 3 shows m_z and p as a function of temperature T for a spin-1 chain of 4 particles with the Hamiltonian (1) for strong interactions $J = 2 \times B$. Both quantities are non-monotonic functions of T and therefore no mapping between m_z and p exists. Note that, although the present plots are done for 4 spins only, the characteristics do not change for larger numbers of spins (The exact quantitative values are not needed for our reasoning). We have studied this with chains of 4, 5 and 6 spins. In the case of m_z, the characteristics have even been already observed in experiments [16].

How could a local observer determine whether the system he observes, a single spin, is in a thermal state and can therefore be characterized by a temperature? The local observer needs
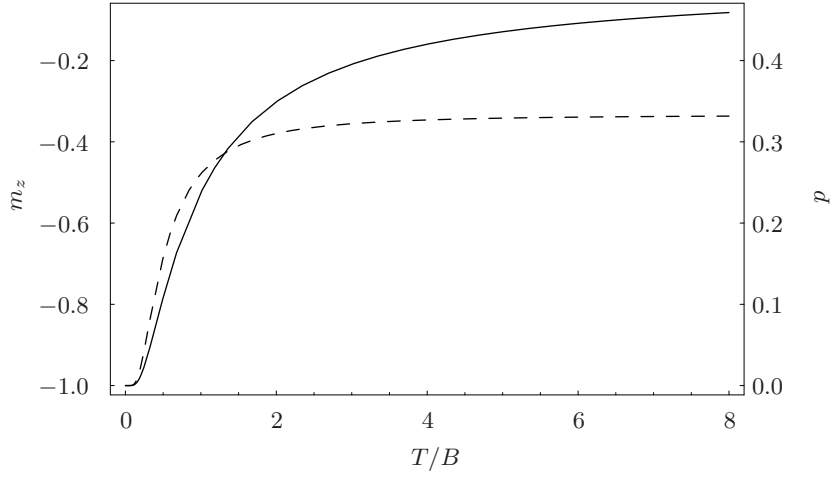
Fig. 2 – m_z (solid line) and p (dashed line) as a function of temperature T for spin-1 chain of 4 particles. T is given in units of B and $J = 0.1 \times B$.

to compare two situations: In the first situation, the spin is weakly coupled to a larger system, the heat bath. In this situation, the local observer could measure m_z and p as functions of the temperature of the heat bath and would get a result similar to figure 2. This result would not be sensitive to the details of the coupling to the heat bath. The local observer would thus recognize this situation as a particular one and might term it the "thermal" situation. The second situation is fundamentally different. The spin is now strongly coupled to its
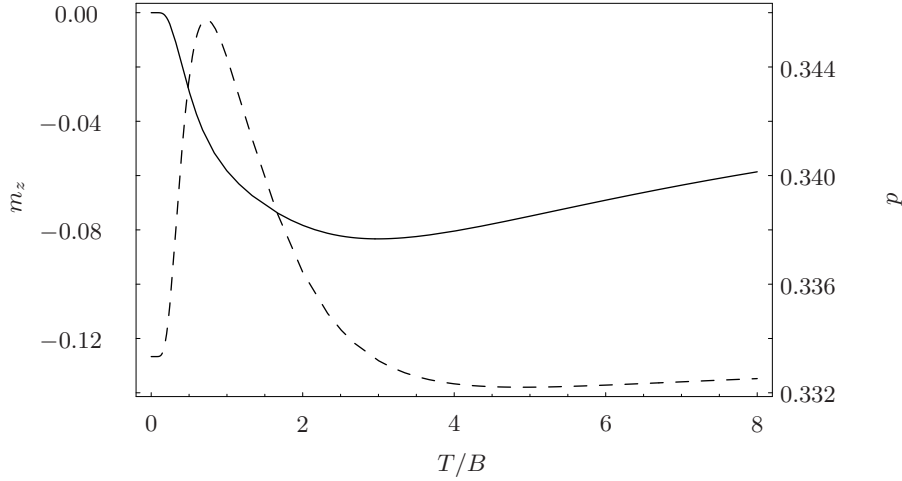

Fig. 3 – m_z (solid line) and p (dashed line) as a function of temperature T for spin-1 chain of 4 particles. T is given in units of B and $J = 2 \times B$.

surrounding. If the local observer again measures m_z and p as functions of the temperature of the surrounding, he gets the result of figure 3.

The observer can tell the difference between both situations, even if he has no access to the temperature T of the surrounding. In the first case he can construct a mapping from say m_z to p or vice versa, in the second he cannot: Here the concept of a local temperature breaks down at least on the level of individual particles, since temperature measurements via different local observables would contradict each other.

Finally, we address the question of whether the effects described here could be observed in real experiments. Indeed, pertinent experiments are available and have partly already been carried out: A realization of a quasi one dimensional anti-ferromagnetic spin-1 Heisenberg chain is the compound CsNiCl$_3$ [14–16]. Here the coupling is $J \approx 2.3$ meV. To achieve a detectable modulation of m_z and p, the spins should be significantly polarized for $T > 0$. Therefore a sufficiently strong applied magnetic field is needed. For CsNiCl$_3$, a field of roughly 9.8 Tesla would correspond to $J = 4 \times B$.

The magnetization in an applied field can be measured with high precision with a SQUID [17]. The occupation probability of the $s_z = 0$ states, on the other hand, is accessible via neutron scattering experiments [18, 19]. The differential cross section for neutron scattering of spin-systems is given by [20]

$$\frac{\partial^2 \sigma}{\partial \Omega \, \partial E_f} \sim \left|f(\vec{q})^2\right| \frac{\left|\vec{k}_f\right|}{\left|\vec{k}_i\right|} \sum_{a,b} \left(\delta_{a,b} - \frac{\vec{q}_a}{|\vec{q}_a|} \cdot \frac{\vec{q}_b}{|\vec{q}_b|}\right) S^{ab}(\vec{q}, \omega), \qquad (8)$$

where E_i, E_f, $\vec{k}_i$ and $\vec{k}_f$ are the initial and final energies and momenta of the scattered neutrons. $a, b = x, y, z$, $\omega = E_f - E_i$, $\vec{q} = \vec{k}_f - \vec{k}_i$ and $f(\vec{q})$ is the magnetic form factor, which can be found tabulated [21]. The dynamic structure factor $S^{ab}(\vec{q}, \omega)$ is the Fourier transform of the spin-spin correlation function,

$$S^{ab}(\vec{q}, \omega) = \frac{1}{2\pi} \int dt \sum_{\vec{r}, \vec{r}'} e^{i\vec{q}(\vec{r}-\vec{r}')-i\omega t} \left\langle \sigma_{\vec{r}}^a(0)\, \sigma_{\vec{r}'}^b(t) \right\rangle. \qquad (9)$$

If we only consider events, where the difference in momentum is along the z-axis, $\vec{q} = q_z \vec{e}_z$, only S^{xx}, S^{xy}, S^{yx} and S^{yy} contribute in equation (8). Since the applied field B is along the z-axis, S^{xy} and S^{yx} are zero due to symmetry reasons. Summing up over all $\vec{q}$ and all ω and using our knowledge of $\vec{k}_i$, $\vec{k}_f$ and $f(\vec{q})$, we can obtain information about the quantity

$$\frac{1}{n} \sum_{\vec{r}} \left\langle \sigma_{\vec{r}}^x(0)\, \sigma_{\vec{r}}^x(0) + \sigma_{\vec{r}}^y(0)\, \sigma_{\vec{r}}^y(0) \right\rangle = 1 + p \qquad (10)$$

from the measurement data. Therefore, p is measurable in neutron scattering experiments. Such experiments or a combination thereof could thus be used to demonstrate the non-existence of local temperature.

We note in passing that such "local" measurements are also an interesting tool to study local and non-local features like entanglement of thermal quantum states [22, 23].

In summary, we have discussed possible "local" temperature measurements via magnetic properties of the considered material. We have studied a magnetic structure in a thermal state and analyzed whether its "local" temperature could be infered from the measurement of magnetic quantities. For a large structure, for which boundary effects can be neglected and thus a model with periodic boundary conditions is a valid description, the magnetization is a

strictly local property implying that a temperature measurement based on it is strictly local, too. Local properties, in general, need not be monotonic functions of the global temperature and thus cannot serve as temperature indicators. The global temperature is not accessible by a local measurement.

For networks of spin-1 or higher dimensional subsystems, two local but different quantities like the magnetization and the occupation probability of the $s_z = 0$ state, cannot be mapped onto each other. As a consequence, using these two quantities for temperature measurements would yield contradictive results. These measurements thus show, that the local state cannot be canonical and that therefore a local temperature does not exist for single spins.

The existence of non-thermal properties within a modular system in thermal equilibrium has so far rarely been recognized. The popularity of a thermal description and the notion of temperature is based on the fact that various properties of the system uniquely scale with temperature. If these mappings do no longer exist, the concept of temperature looses its meaning. This fact might become relevant in future nanotechnologies, in so far as the behavior of a structure can no longer be predicted from a temperature that would characterize it.

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